$1^{c.}\!=\!2\pi$ radians (Donnay & Donnay, 1949). We want to calculate

$$A_{H} = \sum_{n=1}^{N} f_{n} \cos HX_{n}$$
 and $B_{H} = \sum_{n=1}^{N} f_{n} \sin HX_{n}$.

For each of the N atoms in the cell, one card is prepared in which are hand punched: a number j identifying the kind of atom, the running index n, and the co-ordinate X_n of the atom. This master set of N cards is reproduced as many times as there are reflections and, simultaneously, each set has its H value with corresponding $(\sin \theta)/\lambda$ (rounded off to 0.005) gang-punched into it. Then H is multiplied by X_n on the calculating punch (type 602) and the decimal part of the product, rounded off to three places, is punched into the data cards. Sort the cards on HX_{n} and merge with a set of one thousand 'function cards' that carry the values of α , sin α and cos α , from $\alpha = 0.000$ to $\alpha = 0.999$ at intervals of 0.001 cycle. HX_n and α are used as control fields. By intersperse gang-punching the $\cos HX_n$ and $\sin HX_n$ values are transferred from the function cards on to the data cards. Sort on $(\sin \theta)/\lambda$ and on j, an operation which removes the function cards.

Merge each of the j groups of data cards, on $(\sin \theta)/\lambda$ as control field, with the corresponding set of 'f_i cards'. These f_j cards are prepared once and for all; they carry $(\sin \theta)/\lambda$, j, and f_j for $(\sin \theta)/\lambda$ going from 0.000 to 1.500 at intervals of 0.005. The 602 punch is wired to multiply $\cos HX_n$ and $\sin HX_n$ by f_j and to punch the products into the data cards. Finally, sort on H or $(\sin \theta)/\lambda$, depending on the order in which the reflections are to be listed. The tabulator will print for each reflection: $H, (\sin \theta)/\lambda, j, n,$ f_j , the contributions of each atom to A_H and B_H , as well as the sums A_H and B_H .

We wish to thank the Watson Scientific Computing Laboratory for the permission to use their machines and Mr Eric Hankam for his kind assistance in preparing the control panels.

References

DONNAY, J. D. H. & DONNAY, G. H. (1949). Acta Cryst. 2, 366.

DONOHUE, J. & SCHOMAKER, V. (1949). Acta Cryst. 2, 344.

GREMS, M. D. & KASPER, J. S. (1949). Acta Cryst. 2, 347.

Acta Cryst. (1951). 4, 75

Three new polymorphs of silicon carbide, 8H, 75R, and 84R. By L. S. RAMSDELL and J. A. KOHN, Mineralogical Laboratory, University of Michigan, Ann Arbor, Michigan, U.S.A.

(Received 18 October 1950)

Three new polymorphs of silicon carbide have recently been discovered at the Mineralogical Laboratory, University of Michigan. The first of these has an eight-layered hexagonal unit cell, and is designated as type 8H. The crystal is an intergrowth of the new type with the more common 6H. Its structure has been established as having the zig-zag sequence 44 (Ramsdell, 1947). The second polymorph is rhombohedral and has a unit cell of 75 layers. The zig-zag sequence of type 75R is found to be 3232322323 (repeated three times). This structure was deduced by considering sequences involving only the numbers 2, 3 and 4, since no others have been observed in any of the known hexagonal or rhombohedral forms of silicon carbide.

The third polymorph is also rhombohedral and is an intergrowth with type 6H. On the basis of direct measurements on the Weissenberg photographs, it was not absolutely certain whether this new type is 81R or 84R. Using the same empirical limitation mentioned above, the only plausible solution seemed to be an 84-layered unit cell, with a zig-zag sequence of either 33333333232 or 333323332 (each repeated three times). Intensity calculations have proved the first of these arrangements to be the correct one. The fact that the unit cell has 84 layers,

rather than 81, was subsequently verified by the use of a Laue photograph, as suggested by Honjo, Miyake & Tomita (1950). In the Laue photograph, taken with a crystal-to-film distance of 6.5 cm., the resolution of the individual reflections is so much greater than on the Weissenberg films that there is no uncertainty in establishing the 84-layer character of this polymorph.

It will be noticed that neither of these two new rhombohedral types fits into the series proposed by Ramsdell (1947). This suggests the existence of a large number of additional polymorphs, the discovery of which may be effected by continued research. Several Weissenberg photographs obtained recently in our laboratory already indicate some new modifications.

In the near future the authors intend to describe, in a more detailed manner, these three new types of silicon carbide, and to discuss some structural implications of the ever-increasing number of polymorphs of this most unusual compound.

References

HONJO, G., MIYAKE, S. & TOMITA, T. (1950). Acta Cryst. 3, 396.

RAMSDELL, L. S. (1947). Amer. Min. 32, 64.

Acta Cryst. (1951). 4, 75

Concerning reported discrepancies between X-ray and macroscopic measurements of thermal expansion of some alkali halides. By L. F. CONNELL, Jr. and H. C. MARTIN, Jr., Department of Physics, University of Texas, Austin, Texas, U.S.A. (Received 5 September 1950)

A question of fundamental importance in the study of real crystals is the possibility of serious discrepancies in the values of those physical properties, such as thermal expansion, which may be studied by both X-ray and